

Poster Presentation

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Liquid-liquid solvent extraction of rare earths: a crystallographic analysis.

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Liquid-liquid solvent extraction has become the primary research topic for separating mixtures of rare-earths. [1] Current research on this topic focuses on extraction processes involving ionic liquids as basic extracting agents. In the aqueous phase, the rare-earth is coordinated by the anionic entities of the ionic liquid, forming an anionic complex. The large organic cation of the ionic liquid neutralizes the complex (ion-pair complex) and migrates the entity to an organic phase. The choice of these agents is solely based on the calculation of thermodynamical extraction parameters, whilst structural information about these compounds is rare or even non-existent. Our research focuses on obtaining structural information via crystallography on the above-mentioned molecules and relating the interactions between anion and cation to the stability of the complexes. A difference in stability between the anionic complex and cation can give a different extractability. Different rare-earth chloride salts were dissolved in an aqueous phase, containing ionic liquids with β -diketonate anions and 1-alkyl-3-methylimidazolium cations. After the extraction, crystals of the formed compounds are grown from the organic phase and measured. Current results show us that an intermolecular non-classical C-H ... O hydrogen bond is persistent across the different molecules, whilst small interactions between the cation side chain and halogens on the β -diketonate add extra stability to the crystal structure. Structures formed with 2-thenolytrifluoroacetylacetonate anions have no intention to form side chain interactions, leaving the alkyl chain of the 1-alkyl-3-methylimidazolium in a void, whilst structures formed with hexafluoroacetylacetonate have strong side chain interactions, which leads to a better packing. The different solubility of both compounds can be related to the different interactions and stability in the crystal structure.

[1] T. Vander Hoogerstraete, S. Wellens, K. Verachtert, et al., *Green Chemistry*, 2013, 15, 919-927

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